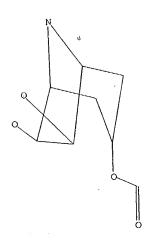
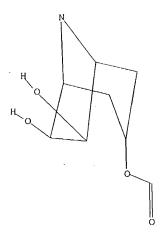
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L2
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L4
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L5
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L6
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L7
              2 S L7 AND PATENT/DT
L8
                S L7 NOT 526-13-6/REG#
     FILE 'REGISTRY' ENTERED AT 19:04:01 ON 24 AUG 2004
              1 S 526-13-6/RN
L9
     FILE 'CAPLUS' ENTERED AT 19:04:01 ON 24 AUG 2004
L10
             86 S L9
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L11
L12
             23 S L11 NOT L8
L13
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L15
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L17
L18
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L19
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Structure attributes must be viewed using STN Express query preparation.

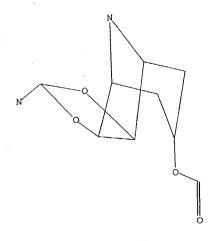
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L4 STR
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10764922



Structure attributes must be viewed using STN Express query preparation.

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=> d bib abs hitstr 1-2
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L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:972072 CAPLUS
DN 140:27968
TI Technical method for producing tropenol
IN Banholzer, Rolf; Bodenbach, Gisela; Mathes, Andreas; Meissner, Helmut; Specht, Peter
```

PA Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany

SO PCT Int. Appl., 21 pp. CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

FAN.	CNT	1																
	PATENT NO.				KIND		DATE		APPLICATION NO.						DATE			
ΡI	WO 2003101986			A1		20031211		WO 2003-EP5158						20030516				
		W:	ΑE,	AG,	ΑL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
			GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
			PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,
			TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	ΑM,	ΑZ,	BY,	KG,	ΚZ,
			MD,	RU,	ΤJ,	TM												
		RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	BG,
			CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	LU,	MC,
			NL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,
			GW,	ML,	MR,	ΝE,	SN,	TD,	TG									
	DE 10224091			A1		20031211		DE 2002-10			1022	0224091			20020531			
US 2003236409						20031225		US 2003-44			4484	48493			20030529			
US 6747153			В2	B2 20040608														
	US 2004158069			A1		20040812		1	US 2	004-	04-764922			20040126				
PRAI	I DE 2002-10224091						2002	0531										
	US 2002-407121P			P		2002	0830											
	US 2003-448493				A1		20030529											
os	OS CASREACT 140:27968;			MAR	PAT	140:	27968	3										
GT																		

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a novel, tech. applicable production method for preparing tropenol (I), optionally in the form of hydrates or acid addition salts, from tropanetriol ester II [R = Cl-4-alkyl, C2-6-alkenyl, Cl-4-alkylene-Ph (optionally substituted with OH or Cl-4-alkoxy)] via reaction with (R'')2NCH(OR')2 (R' = Me, Et; R'' = Me, Et, CH2Et), an elimination reaction of acetals III and deacylation of esters IV. Thus, tiotropium bromide was prepared from meteloidin [II; R = CMe:CHMe-(E)], via reaction with Me2NCH(OMe)2, elimination reaction of acetal III, hydrolysis of ester IV with NaOH in aqueous EtOH, transesterification by I of di(2-thienyl)glycolic acid Me ester, stereoselective epoxidn. with vanadium(V) oxide in DMF, and N-methylation with MeBr.

IT **526-13-6,** Meteloidin

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with DMF di-Me acetal; tech. method for producing tropenol)

RN 526-13-6 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8azabicyclo[3.2.1]oct-3-yl ester, (2E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
     2002:814128 CAPLUS
AN
DN
     137:322727
     Isolation of tropane alkaloid multidrug resistance inhibitors from
     Erythroxylum pervillei and their use for treatment of cancer and
     infections
IN
     Kinghorn, A. Douglas; Pezzuto, John M.
     The Board of Trustees of the University of Illinois, USA
     PCT Int. Appl., 108 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                          KTND
                                  DATE
                                               APPLICATION NO.
                                                                        DATE
PΙ
     WO 2002083669
                           A1
                                  20021024
                                               WO 2002-US11358
                                                                        20020411
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003092729
                                  20030515
                                              US 2002-119874
                           A1
                                                                        20020410
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20040303

EP 2002-762037

BR 2002-8791

20020411

20020411

AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR BR 2002008791 20040309 Α PRAI US 2001-283394P 20010412 P WO 2002-US11358 W 20020411 GΤ

A1

EP 1392685

AR The methods that utilize compds. derived from Erythroxylum pervillei and which modulate the activity of P-glycoproteins are disclosed. The compds. overcome multidrug resistance and can be used therapeutically to enhance performance of therapeutic drugs, like chemotherapeutic drug and antibiotics. Thus, new compds. pervilleine A, B (I), C, D, E, F and A N-oxide were isolated from Erythroxylum pervillei along with two known tropane alkaloid esters; they were characterized by NMR and tested for bioactivity. Pervilleine B (I) was tested for in vitro cytotoxicity against human cancer cell lines [ED50 = $9.4~\mu g/mL$ (BCI); ED50 = 3.1 μ g/mL (Lu1); ED50 = 1.3 μ g/mL (Col2); ED50 = 0.1 μ g/mL (KB-V1+); ED50 = 8.8 μ g/mL (KB-V1-); ED50 = 1.0 μ g/mL (LNCaP); ED50 = 3.2 μ g/mL (SW626)], multidrug resistance [IC50 = 3.8 μ M (SKOV3 ovarian adenocarcinoma); IC50 = >10 μM (BSKVLB ovarian adenocarcinoma); IC50 = 0.12 μ M (SKVLB)] and the relationship of MDR-reversing activity and physicochem. properties [IC50 = >35 μ M (KB-3); IC50 = 15 μ M (KB-V); IC50 = 0.17 μ M (KB-V, done in the presence of vinblastine)].

104086-63-7, Tropane-3 α , 6 β , 7 β -triol

3-phenylacetate

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (isolation, NMR, crystal structure and bioactivity of; tropane alkaloid multidrug resistance inhibitors from Erythroxylum pervillei and their

use for treatment of cancer and infections) 104086--63--7 CAPLUS

Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT => d 1, 5, 10, 15, 20, 23 bib abs hitstr

L12 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:716925 CAPLUS

DN 140:108110

TI Alkaloids of Datura ceratocaula

AU Berkov, Strahil

- CS Department of Applied Botany, Institute of Botany, Bulgarian Academy of Sciences, Sofia, 1113, Bulg.
- SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (2003), 58(7/8), 455-458
 CODEN: ZNCBDA; ISSN: 0939-5075
- PB Verlag der Zeitschrift fuer Naturforschung

DT Journal

LA English

- AB Thirty-six alkaloids were identified in the organs of Datura ceratocaula by GC/MS. Thirty-three of them have not been previously reported for the species. Furthermore, a new tropane ester was tentatively identified as 3-(3'-formyloxytropoyloxy)tropane on basis of its mass spectral fragmentation. Hyoscyamine was the main alkaloid in the plant organs.
- IT 646063-97-0 646063-98-1
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (alkaloids of Datura ceratocaula)

RN 646063-97-0 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (3-endo)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, (2E)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

RN 646063-98-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (3-exo)-6,7-dihydroxy-8-methyl-8azabicyclo[3.2.1]oct-3-yl ester, (2E)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:348260 CAPLUS

DN 137:75928

TI New tropane alkaloids from Erythroxylum moonii

- AU Khattak, Khanzadi Fatima; Atta-ur-Rahman; Choudhary, Mohammad Iqbal; Hemalal, K. D.; Tillekeratne, L. M.
- CS H.E.J. Research Institute of Chemistry, University of Karachi, International Center for Chemical Sciences, Karachi, 75270, Pak.

SO Journal of Natural Products (2002), 65(6), 929-931 CODEN: JNPRDF; ISSN: 0163-3864

PB American Chemical Society

DT Journal

LA English

GΙ

Four new tropane alkaloids were isolated from the leaves of Erythroxylum moonii and identified as 3α -isobutyryloxy- 7β -hydroxynortropane (e.g. I), 3α -hydroxy- 7β -phenylacetoxynortropane, 3α -cis-cinnamoyloxytropane, and 3α -hydroxy- 6β -(3'-hydroxy-2'-methyl-3'-phenylpropionyloxy)- 7β -hydroxytropane. Other alkaloids isolated for the first time from E. moonii were 3α -benzoyloxytropane, 3α -phenylacetoxytropane, 3α -transcinnamoyloxytropane, and 3α -phenylacetoxy- 6β , 7β -dihydroxynortropane. The structures of the new compds. were elucidated by spectroscopic methods.

IT 439791-52-3, 3α -Phenylacetoxy- 6β , 7β -

dihydroxynortropane

RL: BSU (Biological study, unclassified); BIOL (Biological study) (tropane alkaloids from Erythroxylum moonii)

RN 439791-52-3 CAPLUS

CN Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:175556 CAPLUS

DN 112:175556

 ${\tt TI}$ Alkaloids of the genus Erythroxylum. Part 10. Alkaloids of Erythroxylum hypericifolium leaves

AU Al-Said, Mansour S.; Evans, William C.; Grout, Raymond J.

CS Dep. Pharm. Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK

SO Phytochemistry (1989), 28(11), 3211-15 CODEN: PYTCAS; ISSN: 0031-9422

DT Journal

LA English

AB Fifteen alkaloids were characterized from the leaves of E. hypericifolium; the majority are esters of cinnamic and benzoic acids. 3α -Cinnamoyloxytropan-6 β -ol is the main base. New alkaloids reported are 3β -cinnamoyloxytropane, 3α ,6 β -dicinnamoyloxytropane, 3-cinnamoyloxytropane- β -ol, β -acetoxy- β -cinnamoyloxytropane and, tentatively, β -phenylacetoxytropan- β -ol. Two mixed cinnamate dimers were also found. Some syntheses are reported and the chemotaxonomic implications of the results are discussed.

IT 117005-30-8

RN

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of Erythroxylum hypericifolium)

117005-30-8 CAPLUS

CN 2-Propenoic acid, 3-phenyl-, 6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)

GT

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ANSWER 15 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
L12
ΑN
     1979:39083 CAPLUS
     90:39083
DN
ΤI
     Synthesis of betalains
     Buchi, George; Fliri, Hans; Shapiro, Rafael
ΑIJ
     Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA
CS
     Journal of Organic Chemistry (1978), 43(25), 4765-9
SO
     CODEN: JOCEAH; ISSN: 0022-3263
DT
     Journal
     English
LA
```

N-Benzylnorteloidinone (I, R = PhCH2, R1R2 = O, R3 = R4 = H), prepared by Robinson-Schopf synthesis, was converted to the ortho ester I (R = PhCH2 with HC(OMe)3. Catalytic debenzylation of I (R1R2 = O, R3R4 = MeOCH) followed by addition of allylmagnesium bromide gave the carbinol, which was transformed to the I (R = PhCO2, R1 = OH, R2 = H2C:CHCH2, R3R4 = MeOCH) with benzoyl peroxide. Acetylation of the tertiary carbinol was followed by hydrolysis of the ortho ester to the diol. Consecutive oxidns. of the diol to the α -diketone with dimethyl sulfide-N-chlorosuccinimide, and of the olefin to the aldehyde with ozone, gave the diketo aldehyde II. Treatment of II with lead Ph(OAc)4 in MeOH-C6H6 gave a di-Me ester which, upon chromatog. over silica gel, lost both AcOH and BzOH to give di-Me betalamate, characterized by a crystalline semicarbazone (III) of unknown stereochem. Conversion of III to indicaxanthin and betanidin was accomplished using known procedures.

RN 63321-97-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-(benzoyloxy)-3-(2-propenyl)-, 3-acetate, (3-endo,6-exo,7-exo)- (9CI) (CA INDEX NAME)

Ph-C-O N OAC
$$CH_2-CH=CH_2$$

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ANSWER 20 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
L12
AN
      1972:549747 CAPLUS
      77:149747
DN
TI
      Biosynthesis of the isovaleryl and senecioyl moieties of tropane alkaloids
ΑU
      Achari, R. G.; Court, W. E.; Newcombe, F.
      Sch. Org. Chem., Univ. Bradford, Bradford/Yorkshire, UK Planta Medica (1972), 22(1), 38-41
CS
SO
      CODEN: PLMEAA; ISSN: 0032-0943-
ĎΤ
      Journal
LA
      English
```

Incorporation of radioactivity from L-leucine-U-14C and L-valine-U-14C into 8 alkaloids extracted from Datura sanguinea and D. stramonium plants indicated that both amino acids can act as precursors to several isovalery and senecioyl moieties of the tropane alkaloids, including 3-senecioyl-, 3-isovaleryl-, 3, 6-disenecioyl-, and 3, 6-diisovaleryl esters of oxytropane; 3,6-disenecioyl- and 3,6-divalerylesters of oxytropane-7-ol, and 3-senecioyl and 3-isovaleryl- esters of oxytropane-6,7-diol. 38753-89-8 RL: BIOL (Biological study) (formation of isovaleryl moiety of) 38753-89-8 CAPLUS RN Butanoic acid, 3-methyl-, 6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-CN

yl ester (9CI) (CA INDEX NAME)

IT 38753-88-7 RL: BIOL (Biological study) (formation of senecioyl moiety of) RN 38753-88-7 CAPLUS 2-Butenoic acid, 3-methyl-, 6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-CN 3-yl ester (9CI) (CA INDEX NAME)

L12 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN AN 1955:20108 CAPLUS DN49:20108 OREF 49:3987g-i,3988a-e The synthesis of dihydrometeloidine and related compounds TI Sheehan, John C.; Bissell, Eugene R.
Massachusetts Inst. of Technol., Cambridge
Journal of Organic Chemistry (1954), 19, 270-6/
CODEN: JOCEAH; ISSN:-0022-3263 ΑU CS SO DT Journal LA Unavailable AB Dihydrometeloidine (I), structurally related to meteloidine, a natural oxygenated tropane alkaloid, has been synthesized. Teloidinone (II) (3.4 g.) and 4.2 g. p-MeC6 H 4SO3H.H2O in 40 cc. BzH are kept 48 hrs. at 20°, ether is added, the precipitate mixed with 50 cc. N NaOH, and extracted with C6H6, giving 89% benzylideneteloidinone (III), prismatic needles, m. 150-1° [HBr salt, needles, m. 215-16° (decomposition); p-toluenesulfonate, m. 202-3° (decomposition)]. Hydrogenation of 1.95 g. III in 200 cc. 70% EtOH with W-4 Raney Ni at 20° 3-6 hrs. gives 89.5% benzylideneteloidine (IV), needles, m. 163-5° after sublimation at $120^{\circ}/0.05$ mm. [picrate, yellow needles, m. $189-90^{\circ}$ (decomposition); HBr salt, m. $236-7^{\circ}$ (decomposition)]. Adding Na to 260 mg. IV in 25 cc. liquid NH3, until the blue color persists 1 hr., decomposing the mixture with 500 mg. NH4Cl, and evaporating the NH3 give 50 mg. teloidine, m. $166-8^{\circ}$ (decomposition). Treating 1 g. IV with 6 cc. α -methylbutyric anhydride in 6 cc. C5H5N 24 hrs., concentrating the mixture in vacuo, taking up the residue in 25 cc. N HCl, extracting with ether, making the aqueous solution alkaline with 6 cc. 6N NaOH, and again extracting with ether give 61% benzylidene- α -methylbutyrylteloideine (V).HBr, platelets, m. 237.5-8.5° (decomposition) (picrate, yellow needles, m. 161-2°). Hydrogenating 500 mg. V in 10 cc. AcOH with 200 mg. prereduced 30% Pd-C at 20° gives 95.5% I, needles, m. 96-7° [HBr salt, platelets, m. 216-17° (decomposition)]. Treating I g. IV in 6 cc C5H5N with 4 cc. Ac20 24 hrs. at 20° gives 80% benzylideneacetylteloideine (VI), m. 110.5-11.5° [HBr salt, needles, m. 276-7° (decomposition)]. Hydrogenolysis of 500 mg. VI gives 85% acetylteloideine (VII), m.

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178.5-9.5° (decomposition) [HBr salt, m. 207-8° (decomposition)].
Acetylation of teloidine or VII with Ac 20-C5H5N at 20° gives 65%
teloidine triacetate, m. 84.5-5.5°. Treating 260 mg. IV in 10 cc. ether with 220 mg. Ph2C:CO 20 hrs. at 20°, evaporating the mixture, and
neutralizing the residue with HBr give 83\% benzylidenediphenylacetylteloid eine-HBr, platelets, m. 256-7\% (decomposition) [methiodide, m.
205-6° (decomposition)]. Refluxing 3.4 g. II and 4.2 g. p~MeC6H
4SO3H.H2O in 500 cc. Me2CO 24 hrs., adding 100 cc. 0.5N NaOH, evaporating the
Me2CO, and extracting the residual solution with ether give 82.3%
isopropylideneteloidinone (VIII), needles, m. 89-90° [picrate, yellow needles, m. 214-15°; HBr salt, m. 241.5-2.5°;
methiodide, prisms, m. 227-8° (decomposition)]. Hydrogenation of VIII gives 94.3% isopropylideneteloidine (IX), m. 131-3° [HBr salt, needles, m. 195.5-6.5°]. Heating 215 mg. IX with 10 cc. N HCl 15 min. gives teloidine-HCl, m. 307-8° (decomposition).
Isopropylideneacetylteloideine, prepared in 77% yield in the same way as VI,
prismatic needles, m. 73.5-5° [picrate, yellow needles, m. 213-14°; HCl salt, prisons, m. 289-90° (decomposition); HBr salt, needles, m. 295-6° (decomposition)]. Isopropylidenediphenylacetylteloid
eine-HBr m. 165-6.5°; methiodide, needles, m. 211-12°.
Heating 215 mg. IX with 785 mg. BzCl 2 hrs. gives 38%
isopropylidenebenzoylteloideine-HBr, m. 264-5° (decomposition).
Refluxing 3.4 g. II and 4.2 g. p-MeC6H4SO3H.H2O in 500 cc. Me2CO, adding
100 cc. 0.5N NaOH, distilling off the Me2CO in vacuo, concentrating the aqueous solution,
treating the residue with 1.5 g. NaBH4 at 20°, extracting the mixture 24 hrs. with CH2Cl2, and subliming the residue of the CH2Cl2 extract give 50%
isopropylidenepseudoteloidine (X), prisms, m. 121-3° [HCl salt, m. 250-1°; HBr salt, prisms, m. 249-50° (decomposition)].
Hydrolysis of 215 mg. X 15 min. with 10 cc. N HCl gives 87% pseudoteloidine-HCl, m. 265-6^{\circ} (decomposition).
Isopropylideneacetylpseudoteloideine, prepared in 83.7% yield similarly to
VI, m. 125-6.5°.
4074-15-1, Meteloidine, dihydro-
    (and derivs.)
4074-15-1 CAPLUS
1\alpha H, 5\alpha H-Tropane-3\alpha, 6\beta, 7\beta-triol,
3-(2-methylbutyrate) (8CI) (CA INDEX NAME)
```

IT

RN

Relative stereochemistry.

=> d his

(FILE 'HOME' ENTERED AT 18:56:47 ON 24 AUG 2004)

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FILE 'REGISTRY' ENTERED AT 18:57:18 ON 24 AUG 2004
L1 STRUCTURE UPLOADED
L2 5 S L1
L3 167 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 2 S L4 SUB=L3 SAMPLE
L6 38 S L4 SSS FULL SUB=L3
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FILE 'CAPLUS' ENTERED AT 19:01:53 ON 24 AUG 2004
L7
            110 S L6
rs
               2 S L7 AND PATENT/DT
                 S L7 NOT 526-13-6/REG#
     FILE 'REGISTRY' ENTERED AT 19:04:01 ON 24 AUG 2004
L9
               1 S 526-13-6/RN
     FILE 'CAPLUS' ENTERED AT 19:04:01 ON 24 AUG 2004
L10
             86 S L9
             24 S L7 NOT L10
L11
             23 S L11 NOT L8
L12
=> d 2,6,11,16,21 bib abs hitstr
L12 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
     2003:297065 CAPLUS
     140:2784
TΙ
     Nortropane alkaloids from the leaves of Erythoxylum moonii
AH
     Khattak, Khanzadi Fatima; Atta-ur-Rahman; Choudhary, M. Iqbal
     Int. Centre for Chem. Sci., H.E.J., Res. Inst. of Chem., Univ. of Karachi,
     Karachi, 75270, Pak.
     Heterocycles (2003), 60(4), 917-924
     CODEN: HTCYAM; ISSN: 0385-5414
PR
     Japan Institute of Heterocyclic Chemistry
DΤ
     English
LA
AB
     Four new nortropane alkaloids have been isolated from the leaves of
     Erythroxylum moonii and identified as nortropane-3\alpha-6\beta-7\beta-
     triol 3-benzoate 7-(2'-hydroxy-3'-phenylpropanoate) (1),
     nortropane-3\alpha-7\beta-diol 7-trans-cinnamate 3-propanoate (2),
     nortropane-3\alpha-7\beta-diol 7-benzoate 3-(2'-methylpropanoate) (3),
     and nortropane-3\alpha-7\beta-diol 3-(2'-methylpropanoate)
     7-cis-(3'',4'',5''-trimethoxycinnamate) (4). Addnl., five known bases are
     characterized as tropane-3\alpha-7\beta-diol 7-benzoate (5),
     tropane-3\alpha-7\beta-diol 3-phenylacetate (6), tropane-3\alpha-
     7\beta-diol 3-benzoate (7), tropane-3\alpha-6\beta-7\beta-triol
     3-benzoate (8), and tropane-3\alpha-yl 3-(3',4',5'-trimethoxybenzoate)
     (9). The structures for the compds. are proposed on the basis of
     spectroscopic evidences.
     117005-29-5
IT
     RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU
        (nortropane alkaloids from leaves of Erythroxylum moonii)
RN
     117005-29-5 CAPLUS
     8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-methyl-, 3-benzoate,
     (1R, 3-endo, 5S, 6S, 7R)-rel- (9CI) (CA INDEX NAME)
Relative stereochemistry.
 HO
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RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:841082 CAPLUS
 DN 136:131532
 TI Modulation of the Multidrug-Resistance Phenotype by New Tropane Alkaloid Aromatic Esters from Erythroxylum pervillei
 AU Silva, Gloria L.; Cui, Baoliang; Chavez, Daniel; You, Min; Chai, Hee-Byung; Rasoanaivo, Philippe; Lynn, Sean M.; O'Neill, Melanie J.; Lewis, Jane A.; Besterman, Jeffrey M.; Monks, Anne; Farnsworth, Norman R.; Cordell, Geoffrey A.; Pezzuto, John M.; Kinghorn, A. Douglas
 CS Program for Collaborative Research in the Pharmacoutical Sciences and Department of Medicinal Chemistry and Pharmacognosy College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612, USA
 SO Journal of Natural Products (2001); 64(12); 1514-1520

CODEN: JNPRDF; ISSN: 0163-3864

American Chemical Society

DT Journal

LA English

AB Nine tropane alkaloid aromatic esters (1-9) were isolated from the roots of Erythroxylum pervillei by following their potential to reverse multidrug-resistance with vinblastine-resistant oral epidermoid carcinoma (KB-V1) cells. All isolates, including seven new structures (3-9), were evaluated against a panel of human cancer cell lines, and it was found that alkaloids 3 and 5-9 showed the greatest activity with KB-V1 cells assessed in the presence of vinblastine, suggesting that these new compds. are potent modulators of P-glycoprotein. Confirmatory results were obtained with human ovarian adenocarcinoma (SKVLB) cells evaluated in the presence of adriamycin and synergistic studies performed with several cell lines from the NCI tumor panel. The structures of the new compds. were determined using spectroscopic techniques. Single-crystal X-ray anal. was performed on the monoester, tropane- 3α , 6β , 7β -triol 3-phenylacetate (1).

104086-63-7, Tropane-3 α , 6 β , 7 β -triol

3-phenvlacetate

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); BIOL (Biological study); OCCU (Occurrence)

(modulation of the multidrug-resistance phenotype by new tropane alkaloid aromatic esters from Erythroxylum pervillei)

RN 104086-63-7 CAPLUS

Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD RE, CNT 26 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

ΑN 1989:404229 CAPLUS

DN 111:4229

ΤI Alkaloids of the genus Erythroxylum. Part 9. Alkaloids of Erythroxylum hypericifolium stem bark

Al-Said, Mansour S.; Evans, William C.; Grout, Raymond J.

Dep. Pharm. Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK Phytochemistry (1989), 28(2), 671-3 CS

Ş0-CODEN: PYTCAS; ISSN: 0031-9422

DTJournal

LA English

AB Thirteen bases were characterized from the stem bark of E. hypericifolium; hygrine is the principal component. As in the root bark esters of phenylacetic acid predominate; other alkaloids involve acetic, benzoic, and trimethoxycinnamic acids. Alkaloids reported for the first time are 3α -phenylacetoxynortropan- 6β -ol, 6β -acetoxy- 3α -

benzoyloxytropane, and 3-acetoxy-6-phenylacetoxytropane.

IT 104086-63-7

RL: BIOL (Biological study)

(from Erythroxylum hypericifolium stem bark)

RN 104086-63-7 CAPLUS

Benzeneacetic acid, (1R, 3-endo, 5S, 6S, 7R)-6, 7-dihydroxy-8-methyl-8azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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L12
     ANSWER 16 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
     1977:439714 CAPLUS
AN
     87:39714
DN
     Synthesis of betalamic acid
     Buechi, George H.; Fliri, Hans; Shapiro, Rafael
Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA
ΑU
CS
     Journal of Organic Chemistry (1977), 42(12), 2192-4
SO
     CODEN: JOCEAH; ISSN: 0022-3263
DT
     Journal
     English
LA
GΙ
```

MeO₂C
$$\stackrel{\text{NCH}_2\text{Ph}}{\text{HO}}$$
 $\stackrel{\text{NCH}_2\text{Ph}}{\text{HO}}$ $\stackrel{\text{NCH}_2\text{Ph}}{\text{HO}}$ $\stackrel{\text{NO}_2\text{CPh}}{\text{O}}$ $\stackrel{\text{NH}}{\text{CH}_2\text{CH}} = \text{CH}_2$ $\stackrel{\text{NO}_2\text{CPh}}{\text{OH}}$ $\stackrel{\text{NO}_2\text{CPh}}{\text{III}}$ $\stackrel{\text{NO}_2\text{CPh}}{\text{O}_2\text{CMe}}$ $\stackrel{\text{IV}}{\text{IV}}$

AB Betalamic acid dimethyl ester (I) was prepared from N-benzylnorteloidinone (II) via the carbinol III and aldehyde IV in 9 steps.

IT 63321-97-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oxidation of)

RN 63321-97-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-(benzoyloxy)-3-(2-propenyl)-, 3-acetate, (3-endo,6-exo,7-exo)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Ph-C-O & N \\ \hline & HO & N \\ \hline & CH_2-CH=CH_2 \end{array}$$

1968:484182 CAPLUS

69:84182

L12

AN

TТ Alkaloid production in Datura hybrids ΑU Lubis, I. CS Lembaga Biol. Nas., Bogor, Indonesia Annales Bogorienses (1967), 4(3), 163-90 SO CODEN: ABOGAT; ISSN: 0517-8452 DT Journal LA English Alkaloid contents of the roots of Datura hybrid plants of 6 generations, produced by crossing D. ferox and D. stramonium, were determined F-1 generation plants contained hycocyamine (I) 350, hycoscine (II) 160, 3α -tigloyloxytropane (III) 85, meteloidine (IV) 190, 7-hydroxy-3,6-ditigloyloxytropane (V) 400, 3,6-ditigloyloxytropane (VI) 60 mg./kg. of roots, and small amts. of tropane and an unidentified alkaloid. F-5 generation plants contained I 155, II 600, III 300, IV 355, V 200, and VI 77 mg./kg. of roots. All 6 alkaloids were detected in the roots of the

ANSWER 21 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

F2-F5 generation plants, but only I and II were found in the roots of F-6 plants. Unlike the case of the aerial parts of the hybrid plants, where the alkaloid characteristic of the parent D. ferox (high content of II) was dominant, the roots contained a high proportion of I up to the F-4 generation, a characteristic feature of D. stramonium. This difference was due to the inheritance of another independent genetic factor, namely the epoxidizing ability of the aerial parts, which is responsible for the formation of II from I. Variation in the amts. of III, IV, and V in the roots up to the F-5 generation indicated a tendency toward adoption of D. ferox characteristics.

IT 21631-92-5

RL: BIOL (Biological study)
 (in Datura ferox and stramonium)

RN 21631-92-5 CAPLUS

CN $1\alpha H$, $5\alpha H$ -Tropane- 3β , 6β , 7β -triol,

3-(2-methylcrotonate), (E)- (8CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.